Quadratic Optimization: Variant

Last time: we discussed finding the extremal (min & max) values of a quadratic form

$$q(x) = \sum a_{ij} x_i x_j$$

subject to the constraint $1 = \|x\|^2 = x_1^2 + \cdots + x_n^2$.

Procedure: $q(x) = x^T S x$ for S symmetric

orthogonally diagonalize: $S = QDQ^T$ $\quad D = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}$

change variables: $x = Qy$ $\qquad \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$

$$\Rightarrow \quad q(x) = \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2$$

Answer:

maximum $= \lambda_1$, achieved at any unit λ_1-eigenvector

maximum $= \lambda_n$, achieved at any unit λ_n-eigenvector

Here's an (almost) equivalent variant of this problem that you can draw.

Quadratic Optimization Problem, Variant:

Given a quadratic form $q(x)$, find the minimum & maximum values of $\|x\|^2$ subject to $q(x) = 1$.

So we switched the function we're extremizing ($\|x\|^2$) and the constraint ($q(x)=1$).

In general the min/max may not exist.

- $q(x_1,x_2) = -x_1^2 - 2x_2^2$:

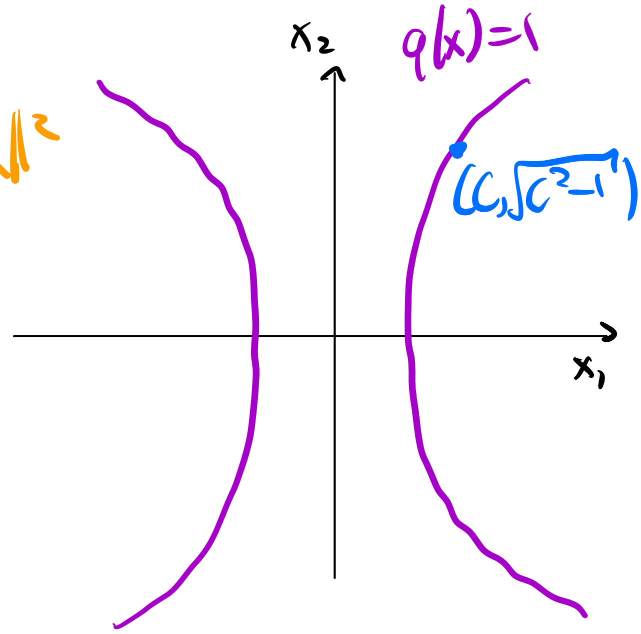
  there is no x such that $q(x)=1$!

- $q(x_1,x_2) = x_1^2 - x_2^2$:

  there is no maximum $\|x\|^2$ subject to $q(x)=1$:

  $$q\left(C, \sqrt{C^2-1}\right) = 1$$

  for any (huge) C.



Problem: $q(x)$ may be 0 or negative!

Def: A quadratic form is positive-definite if $q(x)>0$ for all $x \neq 0$.

NB: If $q(x) = x^T S x$ then q is positive-definite $\iff$ S is positive-definite: this is the positive-energy criterion.

In this case, the problem is equivalent to the previous one, as follows:

Recall: $q(cx) = c^2 q(x)$

Fact: If q is positive-definite then

u maximizes $q(u)$ subject to $\|u\| = 1$ with maximum value λ_1	$\Longleftrightarrow$	$x = \frac{1}{\sqrt{\lambda_1}} u$ minimizes $\|x\|^2$ subject to $q(x)=1$ with minimum value $1/\lambda_1$.

and

u minimizes $q(u)$ subject to $\|u\| = 1$ with minimum value λ_n	$\Longleftrightarrow$	$x = \frac{1}{\sqrt{\lambda_n}} u$ maximizes $\|x\|^2$ subject to $q(x)=1$ with maximum value $1/\lambda_n$

Why? if $q(u) = \lambda > 0$ and $x = \frac{1}{\sqrt{\lambda}} u$ then

$$q(x) = q\left(\frac{1}{\sqrt{\lambda}} u\right) = \frac{1}{\lambda} q(u) = \frac{1}{\lambda} \cdot \lambda = 1.$$

If λ is maximized then $\|x\|^2 = \frac{1}{\lambda}$ is minimized and vice-versa.

So we know exactly how to solve this QO problem variant: do the same procedure as in the original QO problem, and take reciprocals.

Eg: Extremize $\|x\|^2$ subject to

$$q(x_1,x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1x_2 = 1$$

Last time: $q(x) = x^T S x$

$$S = \frac{1}{2}\begin{pmatrix} 5 & -1 \\ -1 & 5 \end{pmatrix} = QDQ^T \quad Q = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \quad D = \begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}$$

- q is maximized (subject to $\|u\|=1$) at $u_1 = \pm\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$ with maximum value 3.

  $$q(u_1) = 3 \quad x_1 = \frac{u_1}{\sqrt{3}} \implies q(x_1) = 1 \quad \|x_1\|^2 = \frac{1}{3}$$

  The minimum value of $\|x\|^2$ subject to $q(x)=1$ is $1/3$. It is achieved at $x_1 = \frac{1}{\sqrt{3}}u_1$.

- q is minimized at $u_2 = \pm\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ with minimum value 2.

  $$q(u_2) = 2 \quad x_2 = \frac{1}{\sqrt{2}}u_2 \implies q(x_2) = 1 \quad \|x_2\|^2 = \frac{1}{2}$$

  The maximum value of $\|x\|^2$ subject to $q(x)=1$ is $1/2$. It is achieved at $x_2 = \frac{1}{\sqrt{2}}u_2$.

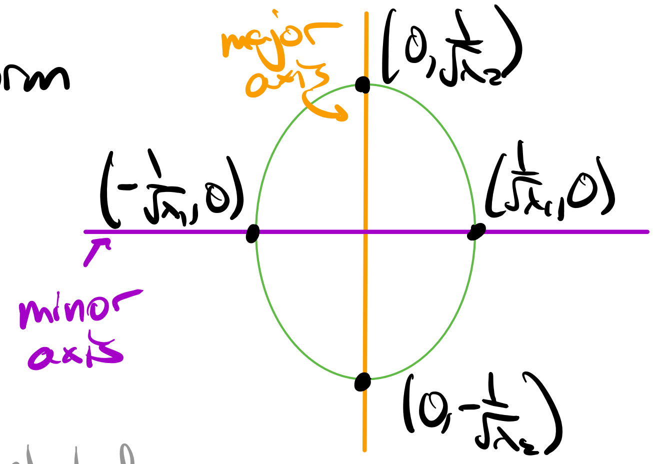
  → note $\frac{1}{2} > \frac{1}{3}$ ✓

Geometric Interpretation

Recall: An equation of the form

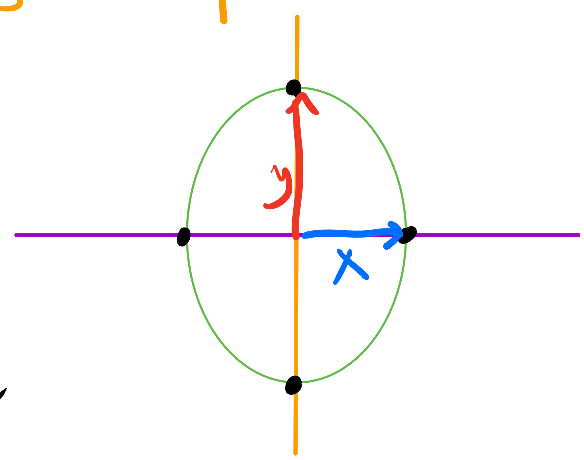
$$\lambda_1 x_1^2 + \lambda_2 x_2^2 = 1$$

$(\lambda_1 \geq \lambda_2 > 0)$ defines an ellipse.



(This is a circle horizontally stretched by $1/\sqrt{\lambda_1}$ & vertically stretched by $1/\sqrt{\lambda_2}$)

If $q(x_1, x_2) = \lambda_1 x_1^2 + \lambda_2 x_2^2$ is diagonal & positive-definite then $q(x_1, x_2) = 1$ defines the ellipse above, and extremizing $\|x\|^2 = 1$ subject to $q(x) = 1$ amounts to finding the shortest $(\pm x)$ & longest $(\pm y)$ vectors on the ellipse.



$\|x\|^2 = 1/\lambda_1$

$\|y\|^2 = 1/\lambda_2$

In general, $q(x) = \lambda_1 x_1^2 + \cdots + \lambda_n x_n^2$ (all $\lambda_i > 0$) defines an ellipsoid ("egg"); extremizing $\|x\|^2$ subject to $q(x) = 1$ means finding the shortest & longest vectors.

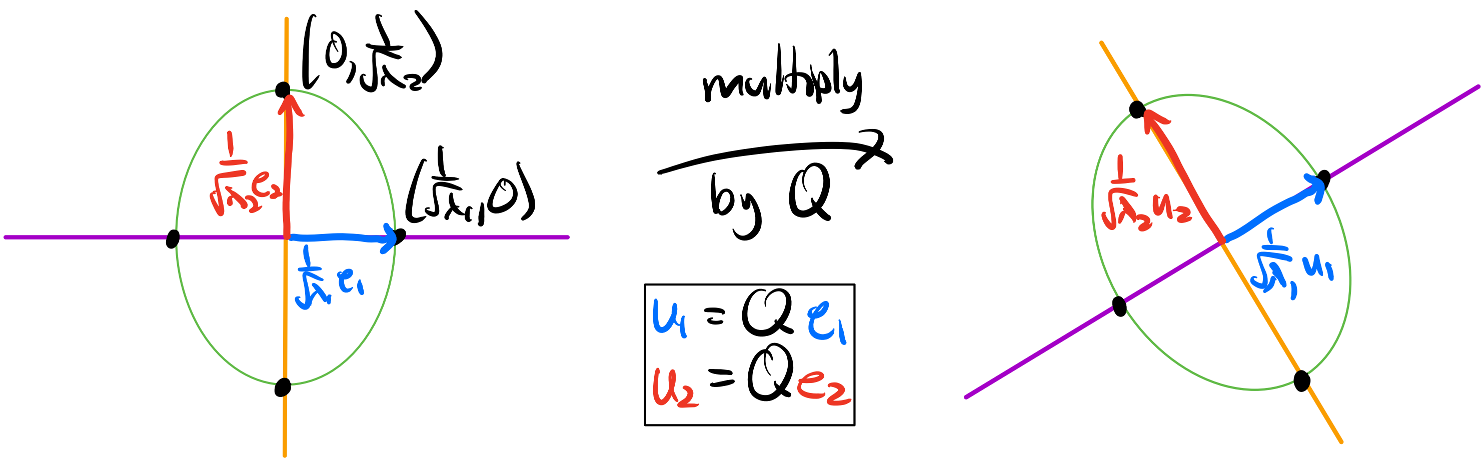
Non-diagonal case:

$q(x) = x^T S x$ for S positive-definite.

Let $\lambda_1 \geq \lambda_2 > 0$ be the eigenvalues, u_1, u_2 orthonormal eigenvectors.

Change variables: $x = Qy$ $\quad Q = \begin{pmatrix} | & | \\ u_1 & u_2 \\ | & | \end{pmatrix}$

$$\lambda_1 y_1^2 + \lambda_2 y_2^2 = 1 \iff q(x) = 1$$



(y_1, y_2)-plane $\qquad$ (x_1, x_2)-plane

Upshot: $q(x) = 1$ defines a (rotated) ellipse.

The minor axis is in the u_1-direction.

$\to$ The shortest vectors are $\pm \frac{1}{\sqrt{\lambda_1}} u_1$

The major axis is in the u_2-direction.

$\to$ The longest vectors are $\pm \frac{1}{\sqrt{\lambda_2}} u_2$.

So we've drawn a picture of quadratic optimization problem (variant).

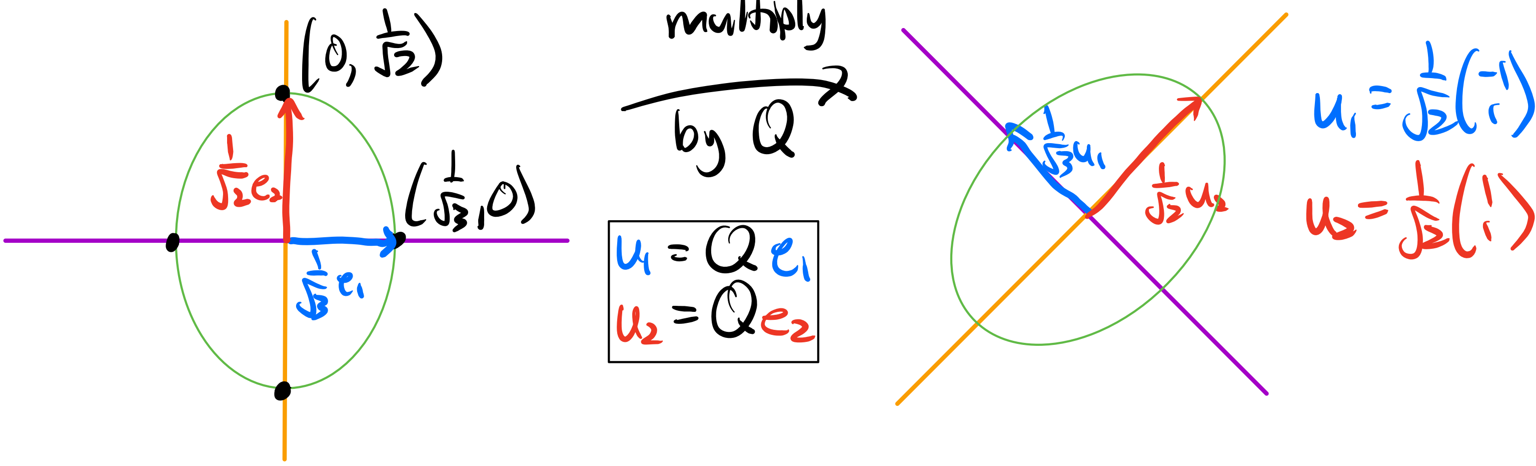
Everything works in higher dimensions; just get rotated ellipsoids.

Eg: $q(x_1, x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1x_2 = x^T S x$

$$S = \frac{1}{2}\begin{pmatrix} 5 & -1 \\ -1 & 5 \end{pmatrix} = QDQ^T \quad Q = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \quad D = \begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}$$

$$x = Qy \rightsquigarrow q = 3y_1^2 + 2y_2^2$$

$3y_1^2 + 2y_2^2 = 1$ $\qquad\qquad$ $q(x) = 1$



(y_1, y_2)-plane $\qquad\qquad$ (x_1, x_2)-plane

The orthogonal diagonalization procedure took the ellipse

$$q(x_1, x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1x_2$$

and found its major & minor axes & radii.

Additional Constraints

These come up naturally in practice (see the spectral graph theory problem on HW13) and in the PCA.

"Second-largest" value:

Suppose $q(x)$ is maximized (subject to $\|x\|=1$) at u_1.
What is the maximum value of $q(x)$ subject to

$$\|x\|=1 \text{ and } x \perp u_1 ?$$

This rules out the maximum value $\rightsquigarrow$ get "second-largest" value.

How to solve this?

- Write $q(x) = x^T S x$
- Orthogonally diagonalize $S = QDQ^T$
  Suppose u_1 is the first column of Q (1st λ_1-eigenvec)
- Set $x = Qy$

  $\rightsquigarrow q = \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2 \qquad \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$

Answer: The maximum value of $q(x)$ subject to $\|x\|=1$ & $x \perp u_1$ is λ_2. It is achieved at any unit λ_2-eigenvector u_2 that is $\perp u_1$.

NB: If $\lambda_1 > \lambda_2$ then $u_2 \perp u_1$ automatically.

Why?

- If $q = \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2$ is diagonal then $u_1 = e_1 = (1, 0, \ldots)$ so $x \perp u_1$ means $y_1 = 0$ is extremizing $\lambda_2 y_2^2 + \lambda_3 y_3^2 + \cdots + \lambda_n y_n^2$.
- Otherwise, change variables $x = Qy$. Q is orthogonal, so

$$y \cdot e_1 = 0 \iff 0 = (Qy) \cdot (Qe_1) = x \cdot u_1$$
$$\|y\| = 1 \iff 1 = \|Qy\| = \|x\|$$

(relate constraints on x & y)

Eg: Find the largest and second-largest values of

$$q(x) = 2x_1^2 + 2x_2^2 + 5x_3^2 + 2x_1x_2 - 8x_1x_3 + 8x_2x_3$$

subject to $x_1^2 + x_2^2 + x_3^2 = 1$.

- $q = x^T S x$ for $S = \begin{pmatrix} 2 & 1 & -4 \\ 1 & 2 & 4 \\ -4 & 4 & 5 \end{pmatrix}$

- $S = QDQ^T$ for

$$Q = \begin{pmatrix} -1/\sqrt{6} & 1/\sqrt{2} & 1/\sqrt{3} \\ 1/\sqrt{6} & 1/\sqrt{2} & -1/\sqrt{3} \\ 2/\sqrt{6} & 0 & 1/\sqrt{3} \end{pmatrix} \qquad D = \begin{pmatrix} 9 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -3 \end{pmatrix}$$

Largest value is $q(x)=9$ at $x=\pm\frac{1}{\sqrt{6}}\begin{pmatrix}-1\\1\\2\end{pmatrix}=\pm u_1$

Second-largest value:

The maximum value of $q(x)$ subject to $\|x\|=1$ & $x\perp u_1$ is

$q(x)=3$ achieved at $x=\pm\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}$

This also works for minimizing.

Second-smallest value:

Suppose $q(x)$ is minimized (subject to $\|x\|=1$) at u_n. What is the minimum value of $q(x)$ subject to $\|x\|=1$ and $x\perp u_n$?

Answer: The minimum value of $q(x)$ subject to $\|x\|=1$ & $x\perp u_n$ is λ_{n-1}. It is achieved at any unit λ_{n-1}-eigenvector u_{n-1} that is $\perp u_n$.

(automatic if $\lambda_{n-1}>\lambda_n$)

You can keep going:

Third-largest value:

Suppose $q(x)$ is maximized (subject to $\|x\|=1$) at u_1 and $q(x)$ is maximized (subject to $\|x\|=1$ and $x \perp u_1$) at u_2.

What is the maximum value of $q(x)$ subject to $\|x\|=1$ and $x \perp u_1$ and $x \perp u_2$?

NB: This "rules out" the largest & second-largest values.

Answer: The maximum value of $q(x)$ subject to $\|x\|=1$ & $x \perp u_1$ & $x \perp u_2$ is λ_3. It is achieved at any unit λ_3-eigenvector u_3 that is $\perp u_1$ and u_2.

(automatic if $\lambda_2 > \lambda_3$)

This also works for the variant problem, except you have to take reciprocals.

Et cetera...

Quadratic Optimization for $S = A^TA$

This is what we'll use for PCA.

Let $S = A^TA$ and $q(x) = x^TSx$. Then

$$q(x) = x^TSx = x^T(A^TA)x = (x^TA^T)(Ax)$$
$$= (Ax)^T(Ax) = (Ax)\cdot(Ax) = \|Ax\|^2$$

$$\boxed{S = A^TA \implies x^TSx = \|Ax\|^2}$$

In this case, extremizing $q(x)$ subject to $\|x\| = 1$ means extremizing $\|Ax\|^2$ subject to $\|x\| = 1$.

Procedure: to extremize $\|Ax\|^2$ subject to $\|x\| = 1$:

Orthogonally diagonalize $S = A^TA$

$\rightsquigarrow$ orthonormal eigenbasis $\{u_1, \ldots, u_n\}$,

eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$.

- The largest value is λ_1, achieved at any unit λ_1-eigenvector u_1.
- The smallest value is λ_n, achieved at any unit λ_n-eigenvector u_n.
- The second-largest value is λ_2, achieved at any unit λ_2-eigenvector $u_2 \perp u_1$. ... etc.

NB: these are eigenvectors/eigenvalues of $S = A^TA$, not of A (which need not be square).

Def: The matrix norm of a matrix A is

$\|A\|$ = the maximum value of $\|Ax\|$ subject to $\|x\| = 1$.

So $\|A\| = \sqrt{\lambda_1}$ λ_1 = largest eigenvalue of A^TA.

Eg: Compute $\|A\|$ for $A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 1 \end{pmatrix}$.

$A^TA = \begin{pmatrix} 3 & 2 \\ 2 & 3 \end{pmatrix}$ $p(\lambda) = \lambda^2 - 6\lambda + 5 = (\lambda-5)(\lambda-1)$

The largest eigenvalue is $\lambda = 5$, so $\|A\| = \sqrt{5}$.

Eigenvector: $\begin{pmatrix} -b \\ a-\lambda \end{pmatrix} = \begin{pmatrix} -2 \\ -2 \end{pmatrix}$

Unit eigenvector: $u_1 = \frac{1}{\sqrt{2^2+2^2}}\begin{pmatrix} -2 \\ -2 \end{pmatrix} = \frac{1}{2\sqrt{2}}\begin{pmatrix} -2 \\ -2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ -1 \end{pmatrix}$

Check: $Au_1 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ -2 \\ -2 \\ -1 \end{pmatrix}$

has length $\frac{1}{\sqrt{2}} \cdot \sqrt{1^2+2^2+2^2+1^2} = \frac{\sqrt{10}}{\sqrt{2}} = \sqrt{5}$ ✓